Size reduction of a semiconductor nanowire laser using metal coating

A. V. Maslov\textsuperscript{a} and C. Z. Ning\textsuperscript{b}

\textsuperscript{a}NASA Ames Research Center, Mail Stop 229-1, Moffett Field, CA 94035, USA;\textsuperscript{b}Department of Electrical Engineering, Arizona State University, Tempe, AZ 95287, USA

ABSTRACT

We explore the possibility of coating semiconductor nanowires with metal (Ag) to reduce the size of nanowire lasers operating at photon energies around 0.8–2 eV. Our results show that the material gain of a typical III-V semiconductor in nanowire may be sufficient to compensate Joule losses of such metal as Ag. The most promising mode to achieve lasing seems to be TM\textsubscript{01} near its cutoff. To calculate the guiding properties of metal coated nanowires, we developed a finite-difference discretization approach, the details of which we also present. This approach allowed us to treat accurately the wire/metal interface and to include nonperturbatively the imaginary parts of dielectric constants of the semiconductor core and metal cladding.

Keywords: nanowires, lasers, waveguide dispersion, plasmons, finite-difference discretization

1. INTRODUCTION

Miniaturization in optoelectronics requires the development of devices with sizes comparable to or smaller than the operating wavelength in vacuum. The size reduction can be achieved using several approaches, from which we will mention just two. The first one is to use waveguides with high dielectric constant surrounded by air. For example, dielectric waveguides can support well-guided modes even for wire radii smaller than the wavelength [1]. This property is now used to make sub-wavelength waveguides using semiconductor or silica nanowires [2, 3]. The second one is to use surface plasmons polaritons guided by metal surfaces that become well localized close to the resonant condition.

Semiconductor lasers and light emitting diodes (LEDs) – the most commonly used devices – can potentially benefit from these two approaches to miniaturization. Indeed, very recently lasing in semiconductor nanowires surrounded by air was demonstrated in ultraviolet (GaN, ZnO), visible (CdS) and infrared (GaSb) spectral ranges [4–7]. At the same time, there is a significant progress in using surface plasmon to achieve lasing. Although the possibility to obtain surface plasmon polariton amplification was suggested in the past [8], recently it attracted significant theoretical [9–11] and experimental interests [12]. The use of non-propagating surface plasmons to make lasers is also being explored [13, 14].

Free standing nanowires have very poor mode confinement at long operating wavelengths, even despite the rather strong dielectric index contrast. The weak confinement also leads to small values of gain and small facets reflections [15, 16]. Thus, one can imagine increasing their confinement by surrounding a nanowire with metal and thus forming core-shell semiconductor-metal waveguide. In such a waveguide the lowest order modes differ from those in a dielectric waveguide or in a metal-wall waveguide operating in the millimeter and centimeter range: they are surface-plasmon polaritons which are localized at the semiconductor/metal interface. However, if the cross-section decreases they lose their evanescent character in the core region and become propagating. These modes are responsible for the operation of near-field scanning optical tips where they are excited by a HE\textsubscript{11} mode of the fiber, but with rather weak efficiency [17]. Here, we investigate the properties of metal-encased nanowires for the purpose of making ultrasmall lasers.

This paper is organized as follows. In Sec. 2 we develop our numerical approach to study the guided properties of cylindrical multi-shell structures. Using this approach we obtain the propagation properties of guided modes and their localization (Sec. 3) as well as modal loss or gain (Sec. 4). In Sec. 4 we draw our conclusions regarding feasibility of using metal encapsulation to decrease the size of nanowire lasers.

Further author information:

A.V.M. is now at Canon Development Americas, Inc., Irvine, CA; e-mail: alexey.maslov@cda.canon.com.
with $\partial \epsilon / \partial \rho$

**Figure 1.** (a) Schematics of a nanowire encased by metal. (b) Grid used for discretization. The labels ±2, ±1, ±0 show the grid points relative to the wire/metal interface; $\Delta \pm$ are grid spacings.

### 2. NUMERICAL APPROACH

Let us consider a semiconductor nanowire encased by metal as shown in Fig. 1(a). To find the guided modes of this structure, we start with Maxwell’s equations and assume that all field behave like $\sim \exp(-i \omega t + ik_z z + i n \varphi)$, where $\omega$ is the frequency of the mode, $k_z$ is its complex propagation wavenumber, $\varphi$ is the angle in the $(x, y)$ plane, $n$ is an integer. While we take $\omega$ as a real number, the propagation number $k_z$ can have both real and imaginary parts, which describe the phase and amplitude $z$–dependence for the modes. Using Maxwell’s equations

$$\nabla \times \mathbf{E} = \frac{i \omega}{c} \mathbf{H}, \quad \nabla \times \mathbf{H} = -\frac{i \omega}{c} \epsilon \mathbf{E}, \quad \nabla \cdot \mathbf{E} = 0$$

in the cylindrical geometry, we reduce them to two equations for the two transverse components ($E_\rho$ and $E_\varphi$) of the electric field:

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial E_\rho}{\partial \rho} \right) - \frac{n^2 + 1}{\rho^2} E_\rho - \frac{2i n}{\rho^2} E_\varphi + \frac{\partial}{\partial \rho} \left( \frac{\epsilon}{\rho^2} \frac{\partial E_\varphi}{\partial \rho} \right) + \frac{\epsilon \omega^2}{c^2} E_\rho = k_z^2 E_\rho$$

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial E_\varphi}{\partial \rho} \right) - \frac{n^2 + 1}{\rho^2} E_\varphi + \frac{2i n}{\rho^2} E_\rho + \frac{\partial}{\partial \rho} \left( \frac{\epsilon}{\rho^2} \frac{\partial E_\rho}{\partial \rho} \right) + \frac{\epsilon \omega^2}{c^2} E_\varphi = k_z^2 E_\varphi.$$  (2)

(3)

In Eqs. (1, 2, 3), $\epsilon = \epsilon(\rho)$ describes the dielectric profile of the waveguide.

Our choice of the field components $E_\rho$ and $E_\varphi$ allowed us to recast the problem of finding waveguide dispersion into an eigenvalue problem defined by Eqs. (2, 3). We solve it by discretizing fields $E_\rho$ and $E_\varphi$ on the grid shown Fig. 1(b). We choose the grid in such a way that all grid points (labeled by $\times$) lie either inside wire or metal. For simplicity, we take uniform grid both in the nanowire (with spacing $\Delta_-$) and metal (with spacing $\Delta_+$). The metal is terminated by the perfect metal boundary condition on the right side. This termination does not affect the guided modes as long as the metal thickness is chosen much greater than the decay length for the modes in the $\rho$-direction. After discretization we arrive at an eigenvalue problem for the vector which consists of values of $E_\rho$ and $E_\varphi$ at the grid points. Since all points lie inside the regions of constant dielectric constant, the terms with $\partial \epsilon / \partial \rho$ in Eqs. (2, 3) vanish but we keep them to obtain the boundary condition at the wire/metal interface.

We discretize the spatial derivatives using

$$\left. \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial f}{\partial \rho} \right) \right|_n = \frac{1}{\Delta^2} \left( \frac{\rho^{n+1/2}}{\rho^n} f^{n+1} - \frac{\rho^{n+1/2} + \rho^{n-1/2}}{\rho^n} f^n + \frac{\rho^{n-1/2}}{\rho^n} f^{n-1} \right)$$

(4)

where the superscripts for all functions denote the values at corresponding grid point; $f$ can be either $E_\rho$ or $E_\varphi$ and $\Delta = \Delta_\pm$ depending on location. This discretization is valid for all points except those that lie next to the origin ($\rho = 0$), interface $\rho = R$ and perfect metal boundary. Below we discuss our approach to writing spatial the derivatives (4) at these points. We start by treating the point that lie next to the origin. We select the grid such that the first point lie exactly a half grid spacing from the origin. This choice conveniently sets $\rho^{n-1/2} = 0$ and the formula (4) remains valid.

We now consider the wire/metal interface ($\rho = R$). We select two virtual grid points which we label as ±0 in Fig. 1(b). The derivatives of $E_\rho$ and $E_\varphi$ at the points near the boundary (±1) can be expressed through the
values of $E_\rho$ and $E_\varphi$ at these two virtual grid points using Eq. (4). On the other hand, the values of $E_\rho$ and $E_\varphi$ at these two points are not defined and should not appear explicitly in discretization. However, they can be expressed via boundary conditions at the interface and the values at the next-to-interface points ($\pm 1$). The boundary conditions follow after integrating Eqs. (2, 3) across the interface and have the following form:

$$
E_\varphi|_{R^+} = 0, \quad \varepsilon E_\rho|_{R^+} = 0, \quad R \frac{\partial E_\varphi}{\partial \rho} + E_\rho|_{R^+} = 0, \quad R \frac{\partial E_\rho}{\partial \rho} - i nE_\rho|_{R^+} = 0.
$$

(5)

To find $E_\rho^\pm$ and $E_\varphi^\pm$ we expand these functions into Taylor series near the interface, for example,

$$
E_\rho(\rho) = \frac{1}{2} \left( 2E_\rho^1 - (E_\rho^0 - E_\rho^{-1})(\rho - \rho^{-1})/\Delta_+ + (E_\rho^0 + 2E_\rho^{-1} + E_\rho^{+1})(\rho - \rho^1)^2/\Delta_+^2, \quad \rho < R \\
2E_\rho^1 + (E_\rho^{+2} - E_\rho^0)(\rho - \rho^1)/\Delta_+ + (E_\rho^{+2} + 2E_\rho^{+1} + E_\rho^0)(\rho - \rho^{+1})^2/\Delta_+^2, \quad \rho > R.
$$

(6)

From the Taylor expansions we can express the derivatives $\partial E_{\rho,\varphi}/\partial \rho$ on both sides of the interface and then use the boundary conditions (5) to express four unknowns $E_\rho^\pm$ and $E_\varphi^\pm$. We obtain:

$$
E_\rho^\pm = \frac{1}{\xi} \left[ \frac{4E_\rho^1 - E_\rho^{+2}}{\Delta_+} - \frac{E_\rho^{-2} - 4E_\rho^{-1}}{\Delta_-} \right],
$$

$$
E_\varphi^\pm = \frac{\eta}{3} \left[ \frac{-E_\varphi^2 + 4E_\varphi^1}{\Delta_+} - \frac{E_\varphi^{-2} - 4E_\varphi^{-1}}{\Delta_-} \right] - 2i \xi \eta \frac{1}{3 \rho} \left( \frac{1}{\varepsilon_+ - 1} - \frac{1}{\varepsilon_-} \right) \left( \frac{4E_\rho^1}{\Delta_+} - \frac{E_\rho^{+2}}{\Delta_+} - \frac{E_\rho^{-2}}{\Delta_-} + \frac{4E_\rho^{-1}}{\Delta_-} \right)
$$

(7)

(8)

where

$$
\frac{1}{\xi} = \frac{1}{\varepsilon_-} \left( \frac{2}{R} + \frac{3}{\Delta_+} \right) - \frac{1}{\varepsilon_+} \left( \frac{2}{R} - \frac{3}{\Delta_+} \right), \quad \frac{1}{\eta} = \frac{1}{\Delta_+} + \frac{1}{\Delta_-}.
$$

(9)

The conditions at the perfect metal boundary are $E_\varphi = 0$, $E_z = 0$. While the first condition can directly be used in the discretization scheme, the second one can be applied to $\nabla \cdot \varepsilon \mathbf{E}$ to give $E_\rho + R\partial E_\rho/\partial \rho = 0$. Expanding $E_\rho$ at the point separated by $\Delta_+$ from the boundary, we obtain the relation between the value of $E_\rho$ at the boundary $E_\rho^0$ and two nearest points $E_\rho^{-1}$, $E_\rho^{-2}$:

$$
E_\rho^0 = \frac{4E_\rho^{-2} - E_\rho^{-1}}{3 + 2\Delta_+/R}.
$$

(10)

where subscripts now denote the distance from the boundary, and not from the $\rho = R$ interface. Since we expressed the values of $E_\rho$ and $E_\varphi$ at the interface $\rho = R$ and at the metal boundary through the values defined on the grid, we can now apply the usual discretization formula (4).

We checked the validity of our numerical scheme by comparing the results for real values of the dielectric constants to those obtained by numerically solving the transcendental dispersion equation [1] and obtained a perfect agreement. The advantage of the using finite discretization with subsequent matrix diagonalization is its simultaneous calculation of all guided modes. This can be easier than searching for roots of transcendental complex dispersions equations, as used for example in Ref. [18]. In addition to that, our choice of grid, in which all points lie within the uniform regions, and the use of rigorous boundary conditions allowed us to treat easily step-index structures avoiding the uncertainty associated with calculating $\partial \varepsilon/\partial \rho$ near the interface. This can also applied directly to multi-shell waveguides. Finally, the numerical diagonalization is particular useful for studying the complex guided modes near their cut-offs, where perturbation techniques fail [19].

3. MODAL PROPERTIES

We start by investigating the guiding properties of the Ag-encased nanowire for purely real values of the dielectric constant of the nanowire. We take $\varepsilon = 12$, a typical value for such commonly used semiconductor as GaAs. The radius is $R = 70$ nm. The dielectric constant of Ag was taken from polynomial approximation [18] and shown in Fig. 2.
Figure 2. Dependence of real and imaginary parts of dielectric constant for Ag on photon energy used in calculations. Note different vertical scales.

Figure 3 shows the dispersions Re $k_z(\omega)$ for nanowires with and without metal. To avoid uncertainty in labeling the modes, we add the superscript “d” when we refer to the modes guided by the nanowire without metal, i.e., purely dielectric waveguide in air. For metal-free nanowires, only two lowest modes ($\text{HE}_{11}$ and $\text{TE}_{11}$) are important. The $\text{TM}_{01}^d$ has typically smaller gain than $\text{TE}_{01}^d$ and will not be discussed here [15]. Although the lowest mode $\text{HE}_{11}$ of an uncoated nanowire does not have a cut-off, its localization inside the wire is very weak for low frequencies. This results in small modal gain and thus, inapplicability of using this mode for making lasers. Thus, if one wants to operate at frequencies below $\sim 1.6$ eV for $R = 70$ nm one can only rely on the modes of Ag-coated wires, in particularly on $\text{HE}_{11}$ and $\text{TM}_{01}$ (see Fig. 3). The $\text{HE}_{11}$ has the smallest cut-off energy and is commonly used to build high-throughput near-field optical probes [17]. Both modes $\text{HE}_{11}$ and $\text{TM}_{01}$ are localized very strongly near the interface at frequencies close to the surface plasmon resonance at about 2.2 eV. This resonant frequency, however, depends on the dielectric constant of the core and can be changed. As the frequency decreases, the mode become propagating in the core, rather than evanescent, after the corresponding dispersions cross the light line (see Fig. 3). At high frequency end, one can also see the usual modes supported by metal waveguides ($\text{EH}_{11}$ and $\text{TE}_{01}$). The phase velocity of these waves, in contrast to $\text{HE}_{11}$ and $\text{TM}_{01}$, is always greater than for plane waves in the core material.

Figure 3. Dependence of the real part of wavenumber on photon energy for a Ag encased nanowire (modes $\text{HE}_{11}$, $\text{EH}_{11}$, $\text{TM}_{01}$, $\text{TE}_{01}$) and the same nanowire in air (modes $\text{HE}_{11}^d$, $\text{TM}_{01}^d$). In both cases the dielectric constant of the nanowire is $\varepsilon = 12$ and radius is $R = 70$ nm.

Having calculated the dispersions, we now turn to the analysis of the spatial distributions of the field components. Figure 4(a) compares the real and imaginary parts of $E_z(\rho)$ for the $\text{TM}_{01}$ at two energies: near the cut-off at 1.55 eV and close to the surface resonance at 2.2 eV. The component $E_z(\rho)$ was obtained by substituting
calculated $E_z(\rho)$ and $E_y(\rho)$ into Maxwell’s equations (1). The presence of metal loss gives rise to the existence of both real and imaginary parts of all field components and $E_z(\rho)$ in particular; without absorption only one (real or imaginary) part would be present. At $E = 2.2$ eV, the field is localized near the interface and decays both in the metal and nanowire. At $E = 1.55$ eV, the field, while still localized near the interface on the metal side, loses its interface localization on the nanowire side. This is related to the propagation character of the field in nanowire near the cutoff when the phase velocity becomes greater than $c/\sqrt{\varepsilon}$.

Figure 4(b) compares the Poynting vectors $S(\rho)$ for metal-encased nanowire (TM$_{01}$ at $E = 1.55$, 2.2 eV) and for metal-free nanowire (HE$_{11}^d$ at $E = 1.55$ eV). We can clearly see that having metal provides a much better localization of the mode. While $S(\rho)$ extends a couple hundred nanometers from the interface for the HE$_{11}^d$, it extends less than 20 nm if metal is used. The ratio of the flux inside nanowire and outside is 1.28/(-0.28) for the TM$_{01}$ and 0.09/0.91 for the HE$_{11}^d$ at $E = 1.55$ eV. The extent of the TM$_{01}$ in the metal depends rather weakly on photon energy in the range from $E = 1.55$ to 2 eV. Near the resonance at $E = 2.2$ eV, $S(\rho)$ in the metal and nanowire have very similar spatial dependences but opposite in sign and practically cancel each other. This results in a very slow group velocity of the resonant surface plasmon polaritons. While $S(z)$ remains negative in metal even for $E = 1.55$ eV, the main part of energy flux is now located in the nanowire; however, the flux still reaches maximum at the interface.

4. GAIN IN METAL-ENCASED NANOWIRES

We know turn to the investigation of loss and gain in metal-encased nanowires. To model gain, we simply add a negative imaginary part to the dielectric constant of the nanowire. We chose three values of the imaginary part of the core semiconductor material: $\varepsilon'' = 0$, -0.1, -0.3. These values of $\varepsilon''$ can be related to the material gain $G$ in the core material by $G = -\omega \varepsilon''/(c \sqrt{\varepsilon})$. For $\varepsilon'' = -0.1$, $E = h\omega = 1.5$ eV, and $\varepsilon = 12$, we obtain $G = 2.2 \times 10^3$ 1/cm. Thus, the values of $|\varepsilon''| \lesssim 0.3$ are within the range attainable in semiconductors.

In the absence of pumping ($\varepsilon'' = 0$), all guided modes have significant Joule loss (see Fig. 3). The HE$_{11}$ and TM$_{01}$ modes have large loss at energies larger than 2 eV due to the surface plasmon resonance. For smaller energies, the loss first decreases but then start to increase. The latter increase is, however, not related directly to Joule loss but rather the manifestation of nonpropagating nature of the mode (see Fig. 3).

As we introduce gain in the core (i.e., introduce a negative $\varepsilon''$), the Im $k_z$ start to decrease, and eventually, we obtain spectral regions with negative Im $k_z$, which corresponds to gain. The decrease of Im $k_z$ with $\varepsilon''$ is greater for the TM$_{01}$ mode than for the HE$_{11}$ mode. This leads to a greater gain for the TM$_{01}$ for $\varepsilon'' = -0.3$ even though initially it has a larger loss.

For TM$_{01}$ at $\varepsilon'' = -0.3$, the whole region near the cutoff becomes negative. Similar behavior is observed for the usual guided mode EH$_{11}$. Just above the cutoff, the gain for the TM$_{01}$ exceed that for the lowest order mode
Figure 5. Dependence of the imaginary parts of wavenumber on photon energy when the nanowire provides gain: imaginary parts of its dielectric constants are $\varepsilon'' = 0$, $-0.1$, $-0.3$. For each mode, lower curves correspond to more negative value of $\varepsilon''$. For $\mathrm{HE}_d^{11}$, the curve for $\varepsilon'' = 0$ is zero and is not shown. The other parameters are the same as for Fig. 3.

$\mathrm{HE}_d^{11}$ of the metal-free semiconductor core. Thus, it is likely that this mode can be used to achieve lasing in metal encased nanowires. On the other hand, the $\mathrm{HE}_d^{11}$ mode can also provide some reasonable values of gain.

Thus, studying the complex dispersion properties of the Ag-encased nanowires we obtained the possibility of obtaining a large negative values of $\text{Im } k_z$ near the low frequency cutoff for the $\mathrm{TM}_{01}$ mode. Just below cut-off, $\text{Im } k_z$ decreases even further but this decrease is not directly related to gain but simply due to non-propagating character of the mode.

5. CONCLUSION

To conclude, we predict the possibility of making ultrasmall lasers made from Ag-encased nanowires. Compared to metal-free nanowires with the same core radius, the operation wavelength is larger. The most promising operational region is near the cutoff for the $\mathrm{TM}_{01}$ mode. Our results are based on exact using experimentally measured properties of Ag and using an accurate finite-difference discretization to calculate the complex dispersion of the waveguide.

To completely evaluate the possibility of lasing using any given mode, one also needs knowledge of the the reflection coefficients to determine the facet losses. For metal-free nanowires the reflections were reported in Ref. [16]. We expect that metal coating can in fact provide a much higher values of the facet reflections. Indeed, the main reason for smallness of the reflection coefficients in metal-free nanowires is the weak mode localization for small radii. In metal, the mode will still be localized very well inside the waveguide. Further, the transverse size of the mode will be smaller than the wavelength in vacuum and, owing to symmetry of $\mathrm{TM}_{01}$, may provide very weak out-coupling (and thus high reflection) for that mode.

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REFERENCES